

Selective extraction of organophosphorous pesticides in plasma by magnetic molecularly imprinted polymers with the aid of computational design

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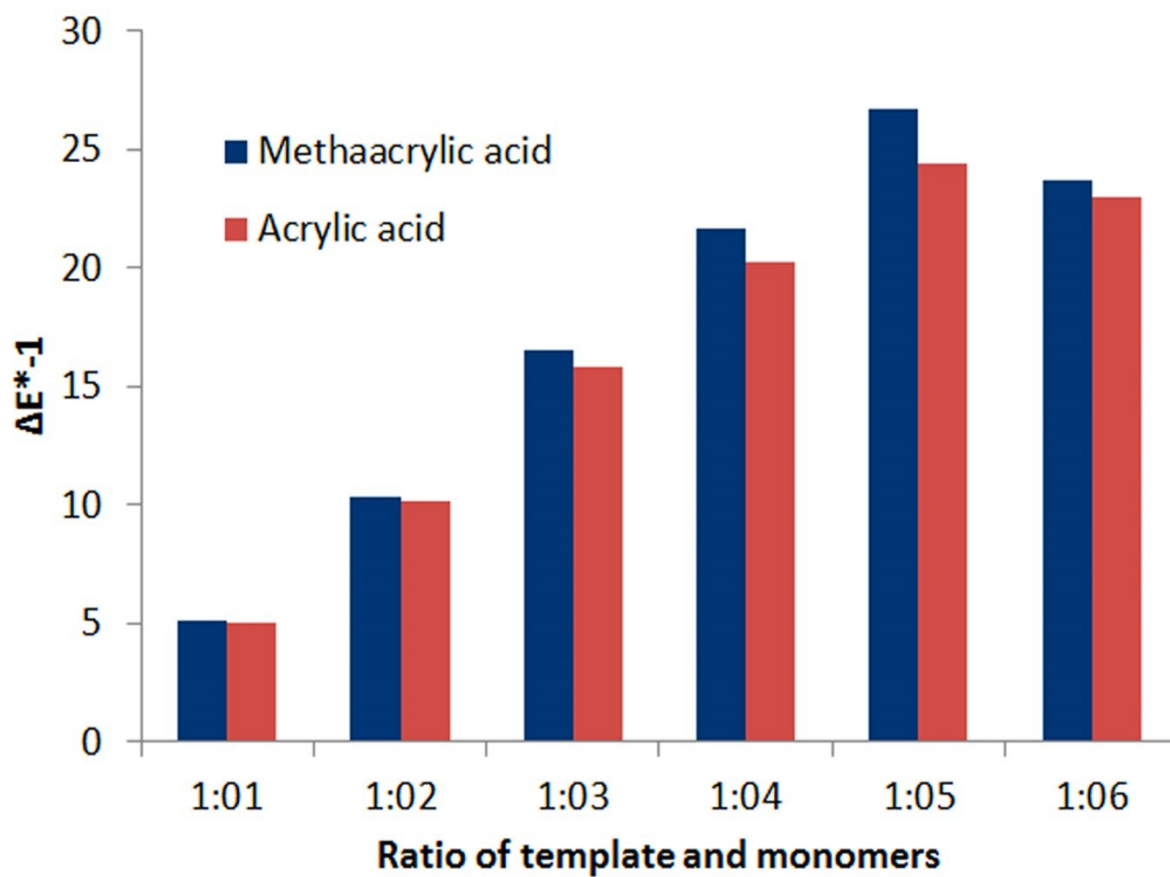


Figure S1. Comparison of interaction energies between template and functional monomers (MAA & AA) at various molar ratios in gas phase

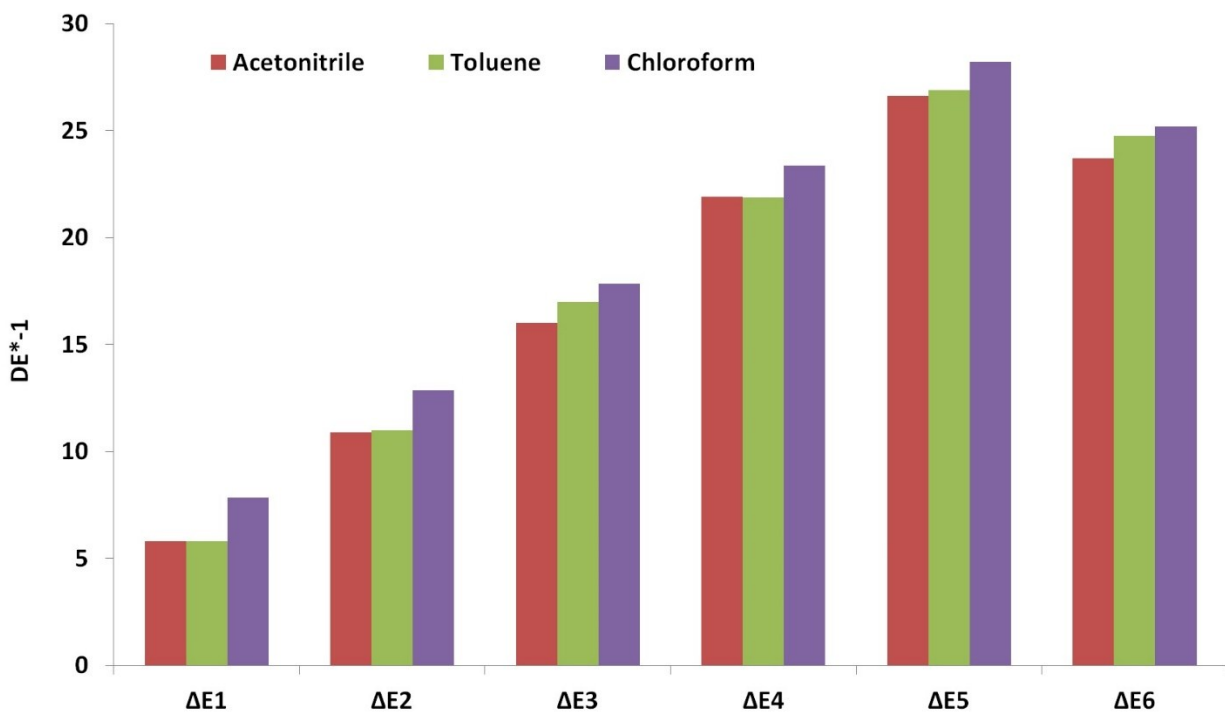


Figure S2. Interaction energies for template functional monomer complexes in various solvents

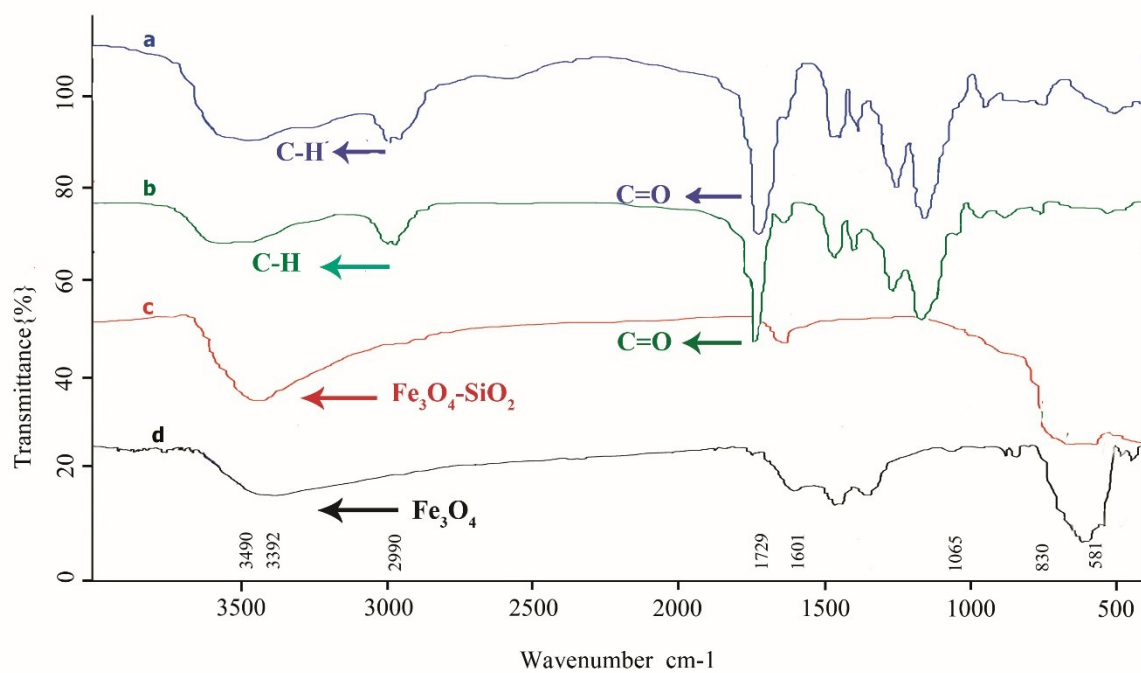


Figure S3. FTIR spectra of MIP-APTES-MNP (a), NIP-APTES-MNP (b), Fe₃O₄NPS (c) and Fe₃O₄-APTES (d).

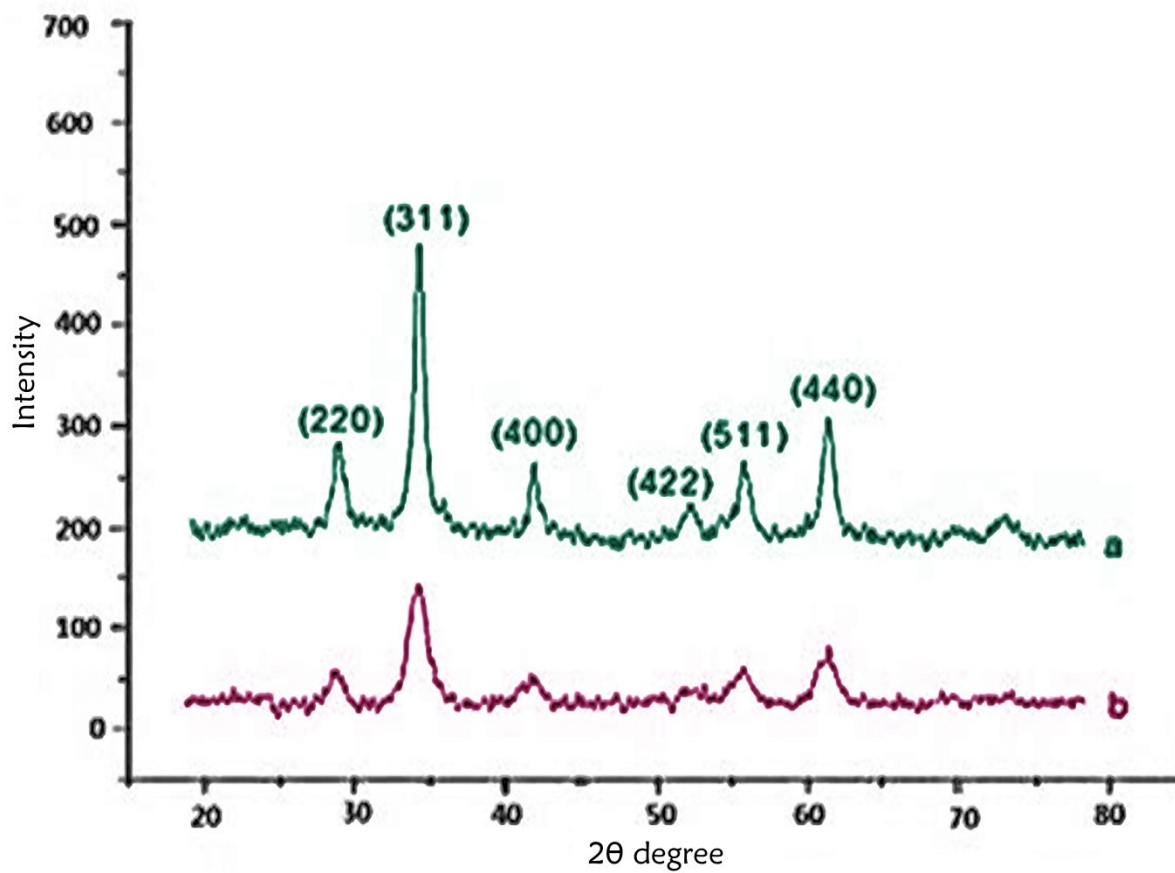


Figure S4. XRD patterns of $\text{Fe}_3\text{O}_4\text{-SiO}_2$ (a), and MIP-APTES-MNP (b)

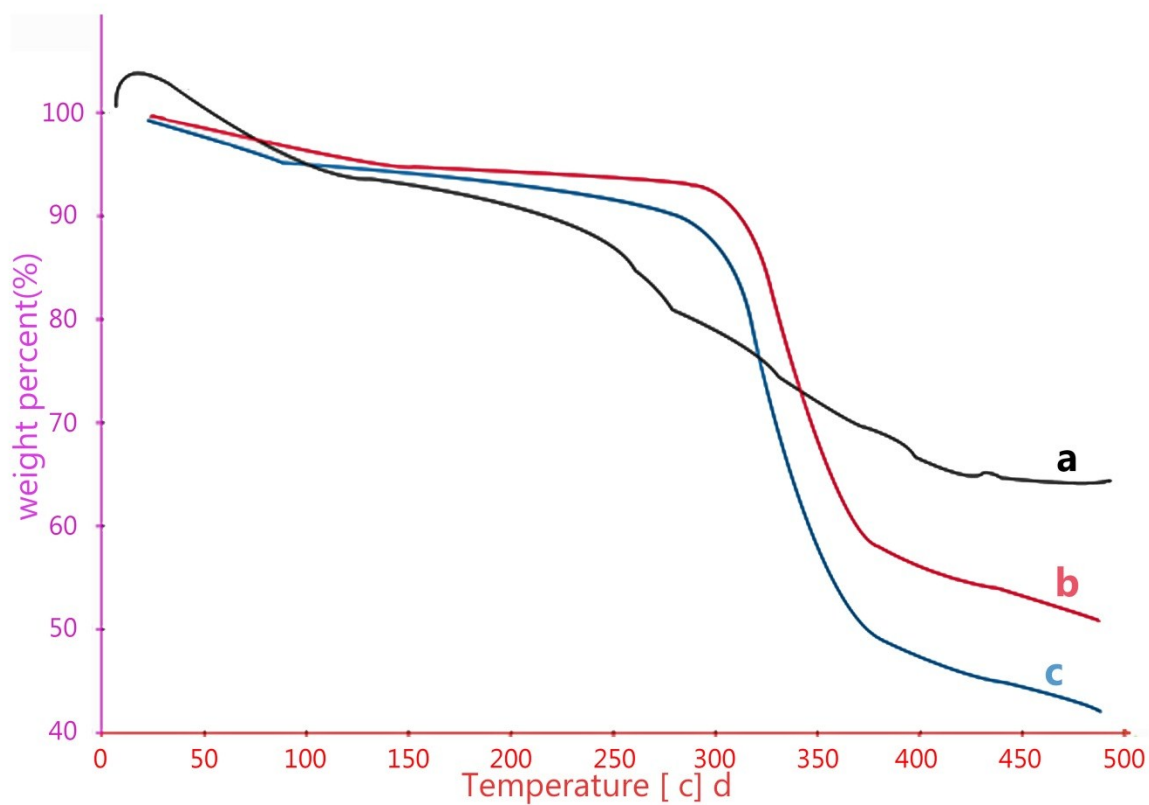


Figure S5. TGA curve of Fe₃O₄-SiO₂ (a), MIP-APTES-MNP (b), and NIP-APTES-MNP (c)

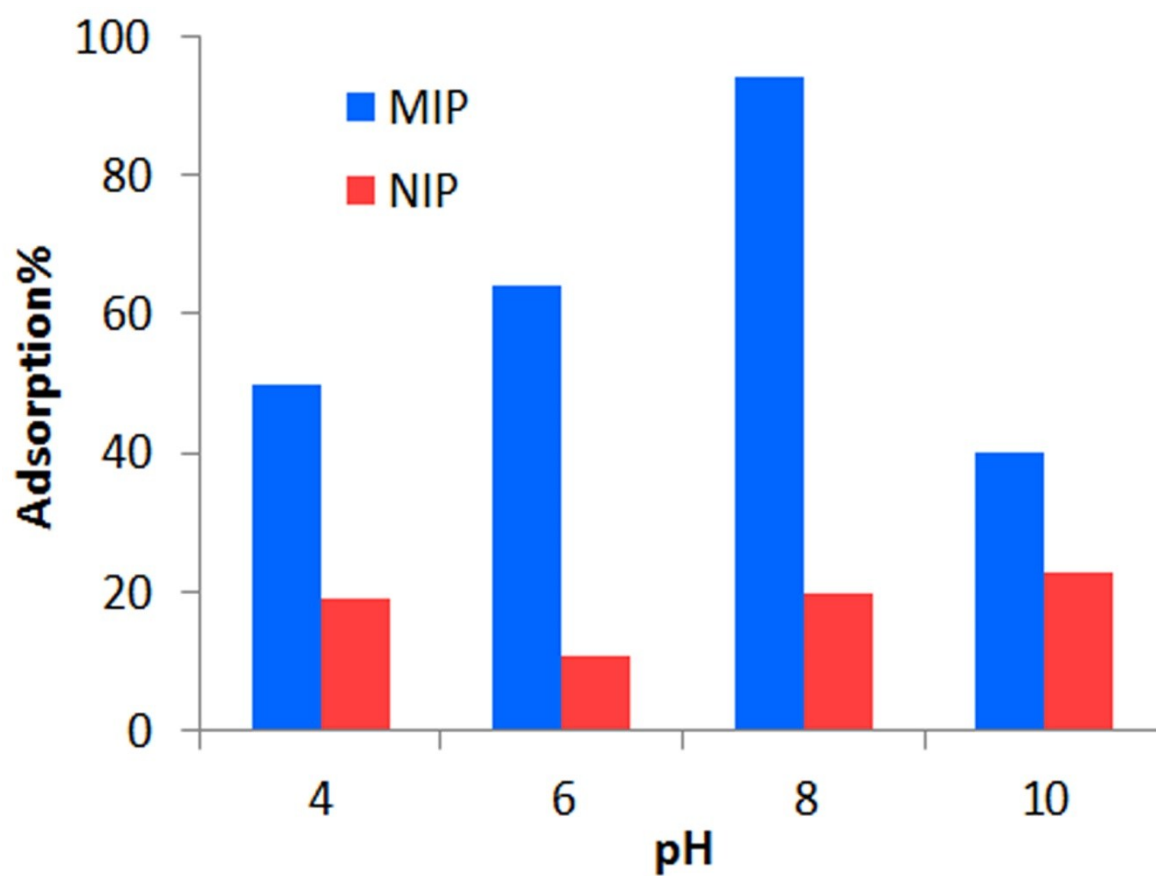


Figure S6. Capacity adsorption of sorbents at different pHs. Experiment condition: 20mg MIP-APTES-MNP and NIP-APTES-MNP at presence of 5ml diazinon solution with 250mg L⁻¹ concentration

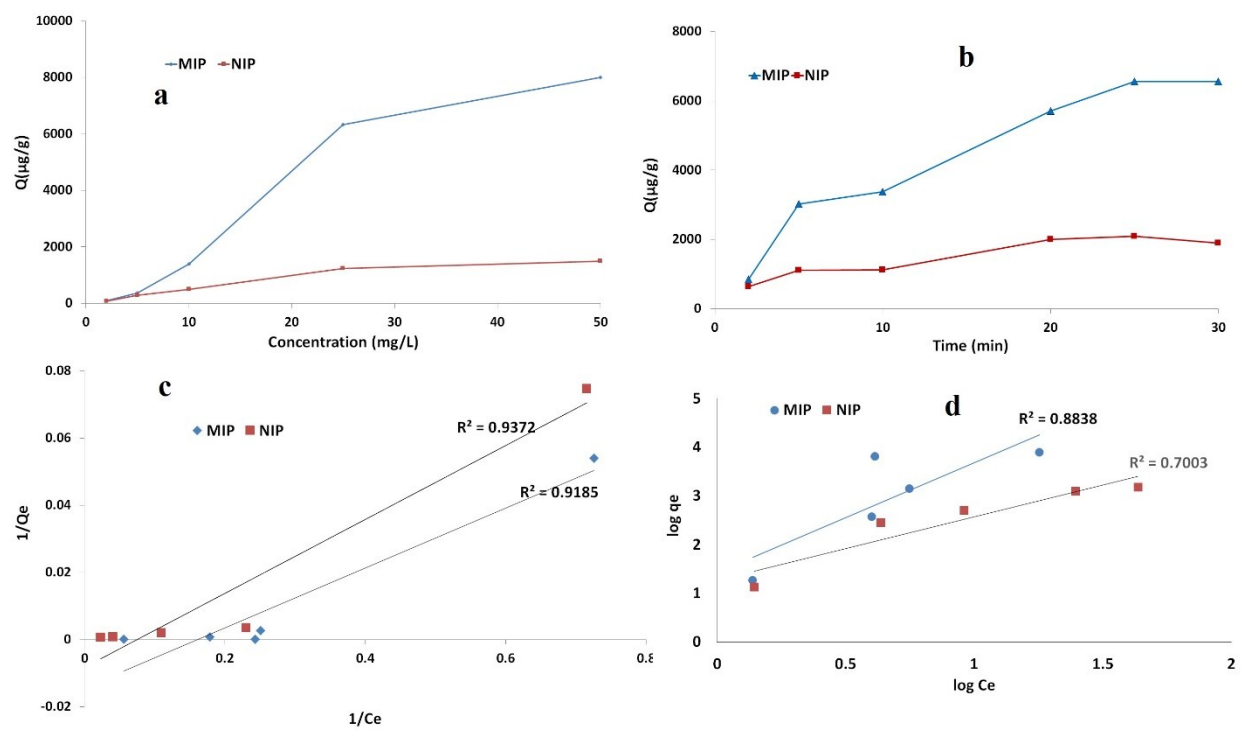


Figure S7. Adsorption profiles; isotherm (a), kinetic (b), Langmuir (c), and Freundlich (d).

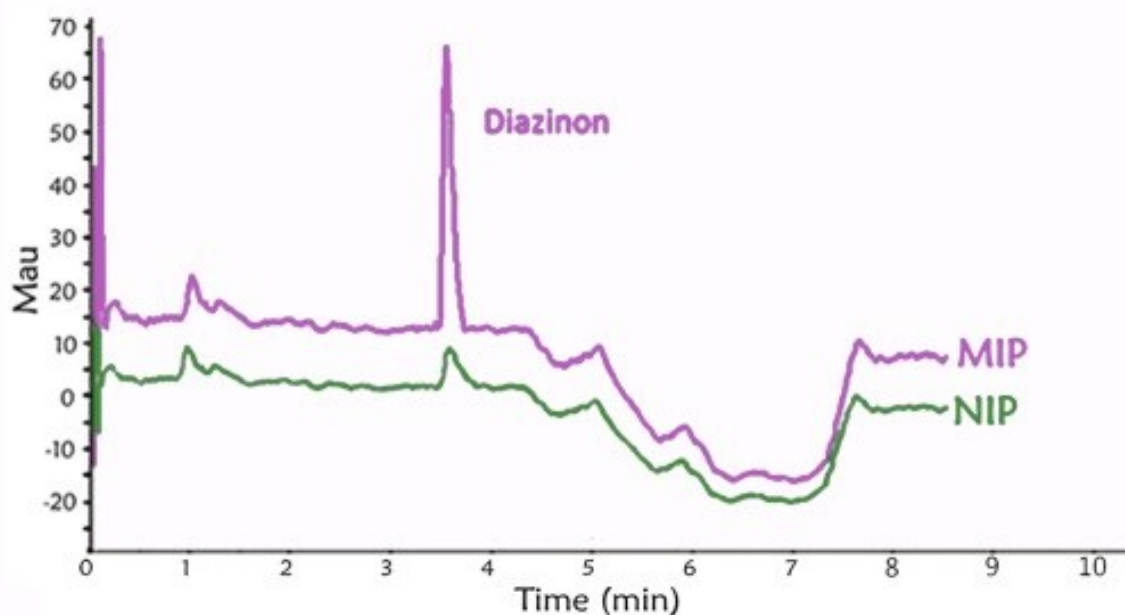


Figure S8 . UHPLC chromatograms obtained after cleaning up and purification of 2ml human plasma spiked with 10 mg/L diazinon using MIP-APTES-MNP(a) and NIP-APTES-MNP(b). Stationary phase: ODS-H C18 (50×2 mm, $1.8 \mu\text{m}$) kept at 25°C . Mobile phase: acetonitril: water (25:75 %v/v) with a flow rate of 1 mL/min.

Table S1. Selectivity parameters of MIP-APTES-MNP and NIP-APTES-MNP for diazinon at the presence of the examined OPPs (* Not applied)

Compound	K_d^{MIP}	K_d^{NIP}	$K_{\text{sel}}^{\text{MIP}}$	$K_{\text{sel}}^{\text{NIP}}$	K
Diazinon	2154.12	43.90	NA*	NA*	NA*
Chlorpyrifose	63.04	30.39	43.37	1.46	23.41
Fosalon	63.08	30.00	19.00	1.21	30.57
Ethion	27.15	19.80	79.34	2.01	40.47
Dichlorvos	147.58	47.5	14.60	1.03	15.85
Malathion	60.41	32.27	36.66	1.36	26.95
Dimethoate	90.23	37.21	24.02	1.18	20.30

Table S2. Linearity parameters, LOD, LOQ and recovery (RR %) of the UHPLC method for chosen OPPs

Pesticide	Equation	R ²	LOD (mg L ⁻¹)	LOQ (mg L ⁻¹)	RR%
Diazinon	Y=10830X-14285	0.9994	0.005	0.016	103
Dichlorvose	Y=12381X-7298.7	0.9966	0.002	0.008	107
Malathion	Y=7012.7X-12885	0.9989	0.007	0.023	101
Dimethoate	Y=11225X-8548	0.9995	0.004	0.013	101
Fosalon	Y=23142X-26519	0.9999	0.002	0.005	99
Chlorpyrifos	Y=12097X-27950	0.9967	0.008	0.028	101
Ethion	Y=14691X-48236	0.9994	0.004	0.014	96